



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:37 am BST

PDB ID : 4BFF
Title : Superoxide reductase (Neelaredoxin) from *Archaeoglobus fulgidus* in the reduced form
Authors : Bandejas, T.M.; Rodrigues, J.V.; Sousa, C.M.; Barradas, A.R.; Pinho, F.G.; Pinto, A.F.; Teixeira, M.; Matias, P.M.; Romao, C.V.
Deposited on : 2013-03-18
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

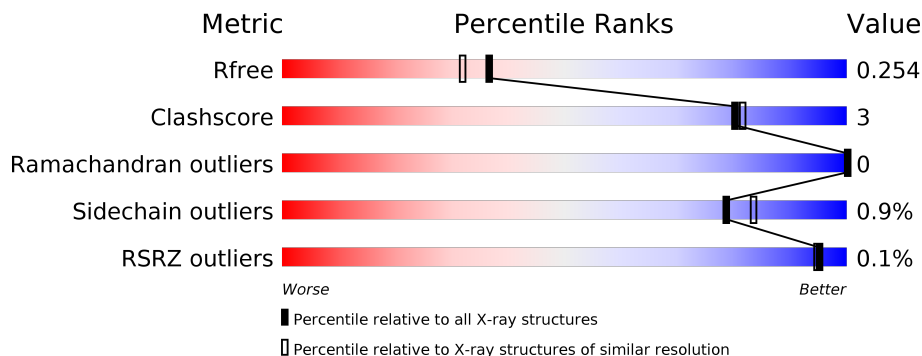
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



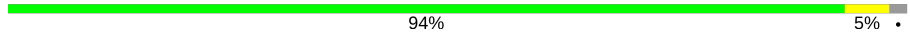


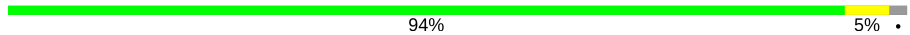


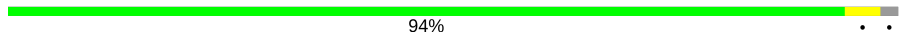



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	125	94%
1	B	125	90%
1	C	125	97%
1	D	125	91%
1	E	125	94%
1	F	125	97%

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Mol	Chain	Length	Quality of chain
1	G	125	 94% 5% .
1	H	125	 90% 8% .
1	I	125	 93% 6% .
1	J	125	 94% 5% .
1	K	125	 93% 6% .
1	L	125	 91% 6% ..
1	M	125	 94% . .
1	N	125	 90% 9% .
1	O	125	 94% 6% .
1	P	125	 89% 10% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16742 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SUPEROXIDE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	123	963	625	159	177	2	3	2	0
1	B	123	951	616	158	175	2	1	0	0
1	C	124	961	621	159	179	2	5	0	0
1	D	123	951	616	158	175	2	1	0	0
1	E	123	951	616	158	175	2	2	0	0
1	F	123	959	621	161	175	2	5	1	0
1	G	123	951	616	158	175	2	3	0	0
1	H	123	951	616	158	175	2	5	0	0
1	I	123	951	616	158	175	2	1	0	0
1	J	123	951	616	158	175	2	3	0	0
1	K	123	961	624	158	177	2	1	2	0
1	L	123	955	620	158	175	2	0	1	0
1	M	123	951	616	158	175	2	1	0	0
1	N	123	957	620	158	177	2	1	1	0
1	O	124	961	621	159	179	2	0	0	0
1	P	123	955	620	158	175	2	1	1	0

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0
2	J	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	K	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	N	1	Total Fe 1 1	0	0
2	O	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0
2	M	1	Total Fe 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	103	Total O 103 103	0	0
3	B	99	Total O 99 99	0	0
3	C	114	Total O 114 114	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	82	Total 82	O 82	0	0
3	E	87	Total 87	O 87	0	0
3	F	100	Total 100	O 100	0	0
3	G	87	Total 87	O 87	0	0
3	H	61	Total 61	O 61	0	0
3	I	118	Total 118	O 118	0	0
3	J	89	Total 89	O 89	0	0
3	K	83	Total 83	O 83	0	0
3	L	78	Total 78	O 78	0	0
3	M	99	Total 99	O 99	0	0
3	N	84	Total 84	O 84	0	0
3	O	90	Total 90	O 90	0	0
3	P	72	Total 72	O 72	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: SUPEROXIDE REDUCTASE

Chain A:  94%



- Molecule 1: SUPEROXIDE REDUCTASE

Chain B:  90%

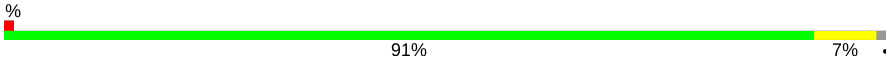


- Molecule 1: SUPEROXIDE REDUCTASE

Chain C:  97%



- Molecule 1: SUPEROXIDE REDUCTASE

Chain D:  91%



- Molecule 1: SUPEROXIDE REDUCTASE

Chain E:  94%



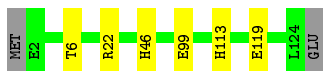
- Molecule 1: SUPEROXIDE REDUCTASE

Chain F:  97%



- Molecule 1: SUPEROXIDE REDUCTASE

Chain G: 94% 5%



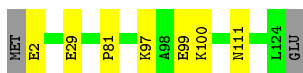
- Molecule 1: SUPEROXIDE REDUCTASE

Chain H: 90% 8%



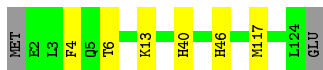
- Molecule 1: SUPEROXIDE REDUCTASE

Chain I: 93% 6%



- Molecule 1: SUPEROXIDE REDUCTASE

Chain J: 94% 5%



- Molecule 1: SUPEROXIDE REDUCTASE

Chain K: 93% 6%



- Molecule 1: SUPEROXIDE REDUCTASE

Chain L: 91% 6%

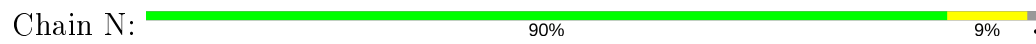


- Molecule 1: SUPEROXIDE REDUCTASE

Chain M: 94%



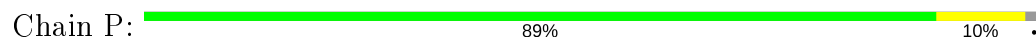
- Molecule 1: SUPEROXIDE REDUCTASE



- Molecule 1: SUPEROXIDE REDUCTASE



- Molecule 1: SUPEROXIDE REDUCTASE



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.32Å 100.23Å 109.68Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	48.11 – 2.00 48.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.0 (48.11-2.00) 89.5 (48.11-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.206 , 0.254 0.206 , 0.254	Depositor DCC
R_{free} test set	6526 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtrriage
Anisotropy	0.841	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.023 for -k,-h,-l 0.022 for k,h,-l 0.358 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16742	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3466e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/997	0.54	0/1355
1	B	0.39	0/979	0.53	0/1332
1	C	0.39	0/989	0.56	0/1344
1	D	0.39	0/979	0.49	0/1332
1	E	0.36	0/979	0.50	0/1332
1	F	0.37	0/990	0.52	0/1346
1	G	0.39	0/979	0.52	0/1332
1	H	0.36	0/979	0.51	0/1332
1	I	0.40	0/979	0.50	0/1332
1	J	0.39	0/979	0.52	0/1332
1	K	0.40	0/995	0.51	0/1354
1	L	0.40	0/986	0.56	0/1342
1	M	0.38	0/979	0.53	0/1332
1	N	0.39	0/988	0.53	0/1344
1	O	0.39	0/989	0.51	0/1344
1	P	0.38	0/986	0.53	0/1342
All	All	0.39	0/15752	0.52	0/21427

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	963	0	947	3	0
1	B	951	0	928	10	0
1	C	961	0	934	0	0
1	D	951	0	928	8	0
1	E	951	0	928	4	0
1	F	959	0	941	1	0
1	G	951	0	928	5	0
1	H	951	0	928	9	0
1	I	951	0	928	5	0
1	J	951	0	928	3	0
1	K	961	0	943	4	0
1	L	955	0	937	6	0
1	M	951	0	928	3	0
1	N	957	0	934	7	0
1	O	961	0	934	6	0
1	P	955	0	937	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	103	0	0	1	0
3	B	99	0	0	7	0
3	C	114	0	0	1	0
3	D	82	0	0	3	1
3	E	87	0	0	4	0
3	F	100	0	0	2	0
3	G	87	0	0	4	0
3	H	61	0	0	4	0
3	I	118	0	0	4	1
3	J	89	0	0	0	0
3	K	83	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	78	0	0	5	0
3	M	99	0	0	1	0
3	N	84	0	0	3	0
3	O	90	0	0	3	0
3	P	72	0	0	1	0
All	All	16742	0	14931	81	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2062:HOH:O	1:H:68:ARG:NH2	1.95	0.99
3:B:2068:HOH:O	1:D:68:ARG:NH1	2.04	0.90
1:L:79:ASP:OD1	3:L:2057:HOH:O	1.90	0.88
1:A:2:GLU:OE2	3:A:2005:HOH:O	1.91	0.86
3:O:2077:HOH:O	1:P:85:GLY:O	1.94	0.85
1:G:6:THR:OG1	3:G:2007:HOH:O	1.96	0.82
1:L:37:GLU:OE1	3:L:2032:HOH:O	2.00	0.79
1:E:19:GLU:OE1	3:E:2015:HOH:O	2.00	0.79
1:B:99:GLU:HG2	1:B:100:LYS:HG3	1.63	0.78
1:G:99:GLU:OE2	3:G:2077:HOH:O	2.04	0.74
1:B:97:LYS:NZ	3:B:2086:HOH:O	2.20	0.73
1:O:99:GLU:O	3:O:2080:HOH:O	2.06	0.72
1:I:81:PRO:O	3:I:2088:HOH:O	2.08	0.71
1:B:36:LYS:NZ	3:B:2038:HOH:O	2.22	0.71
3:N:2055:HOH:O	1:P:52:GLU:OE2	2.08	0.71
1:E:31:LYS:NZ	3:E:2023:HOH:O	2.24	0.71
1:E:89:ASP:OD2	3:E:2066:HOH:O	2.11	0.67
1:L:99:GLU:OE2	3:L:2064:HOH:O	2.13	0.66
1:O:2:GLU:N	3:O:2002:HOH:O	2.27	0.66
3:N:2054:HOH:O	1:P:65[A]:VAL:HG21	1.94	0.66
1:H:11:LYS:O	3:H:2007:HOH:O	2.14	0.66
1:I:29:GLU:OE2	3:I:2042:HOH:O	2.12	0.65
1:L:68:ARG:NH1	1:L:70:GLU:OE2	2.31	0.64
1:E:7:ALA:O	3:E:2004:HOH:O	2.15	0.63
1:G:119:GLU:OE2	3:G:2080:HOH:O	2.14	0.63
1:D:97:LYS:HG2	3:D:2066:HOH:O	1.98	0.63
1:N:24:GLU:O	1:N:27:VAL:HG12	1.99	0.62
3:M:2095:HOH:O	1:O:2:GLU:OE2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:SER:OG	3:H:2049:HOH:O	2.10	0.60
1:D:33:SER:HB2	3:D:2025:HOH:O	2.01	0.60
1:M:8:ASP:HB3	1:M:11:LYS:HG2	1.85	0.59
1:D:2:GLU:OE2	3:D:2001:HOH:O	2.17	0.58
1:A:8:ASP:OD2	1:A:10:LYS:NZ	2.39	0.54
1:L:103:LYS:HE3	1:L:119:GLU:HB3	1.88	0.54
1:B:10:LYS:NZ	3:B:2018:HOH:O	2.40	0.54
1:F:31:LYS:NZ	3:F:2029:HOH:O	2.36	0.53
1:D:52:GLU:HG3	1:D:68:ARG:HB2	1.89	0.53
1:N:109:TYR:CE2	1:P:65[A]:VAL:HG22	2.46	0.51
1:J:40:HIS:CE1	1:J:46:HIS:NE2	2.78	0.50
1:J:4:PHE:HB3	1:J:117:MET:HG2	1.94	0.50
1:M:63:PRO:HG3	1:O:3:LEU:HD22	1.93	0.50
1:I:111:ASN:HB2	3:L:2053:HOH:O	2.12	0.50
1:K:22:ARG:NH1	3:K:2022:HOH:O	2.40	0.50
1:N:52[A]:GLU:HG3	1:N:107:PHE:HB2	1.93	0.50
1:N:109:TYR:CZ	1:P:65[A]:VAL:HG22	2.46	0.50
1:P:8:ASP:HB3	1:P:11:LYS:HE3	1.95	0.49
1:N:55:PHE:CE2	1:N:57:PRO:HG3	2.47	0.49
1:O:2:GLU:HG3	1:O:4:PHE:H	1.78	0.48
1:I:97:LYS:NZ	3:I:2101:HOH:O	2.30	0.48
1:A:22:ARG:NH1	1:A:29[B]:GLU:OE1	2.47	0.48
1:H:24:GLU:O	1:H:27:VAL:HG12	2.14	0.47
1:D:2:GLU:HG3	1:D:4:PHE:H	1.79	0.47
1:N:11:LYS:NZ	3:N:2020:HOH:O	2.48	0.47
1:H:100:LYS:HD2	3:H:2033:HOH:O	2.15	0.46
1:B:37:GLU:O	3:B:2053:HOH:O	2.20	0.46
1:H:26:GLY:O	1:H:97:LYS:HD3	2.16	0.46
1:P:3:LEU:HA	1:P:3:LEU:HD23	1.74	0.46
1:B:63:PRO:HG3	1:D:3:LEU:HD22	1.98	0.44
1:G:22:ARG:NH2	3:G:2022:HOH:O	2.51	0.44
1:O:68:ARG:NH1	1:O:70:GLU:OE2	2.51	0.44
1:N:48:ILE:HB	1:N:90:PRO:HB3	2.00	0.44
1:H:8:ASP:HB3	1:H:11:LYS:HG2	2.00	0.43
1:L:31:LYS:NZ	3:L:2030:HOH:O	2.49	0.43
1:P:4:PHE:HB3	1:P:117:MET:HG2	1.99	0.43
1:K:23:ALA:HB1	1:K:124:LEU:HD23	1.99	0.43
1:B:9:TRP:CZ3	1:B:36:LYS:HD3	2.54	0.43
1:M:21:LEU:HD11	1:M:31:LYS:HB2	2.00	0.43
1:B:55:PHE:CE2	1:B:57:PRO:HG3	2.54	0.43
1:P:103:LYS:HE3	1:P:119:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2094:HOH:O	1:D:93:VAL:HG13	2.19	0.42
1:K:13:LYS:HD3	1:K:40:HIS:HA	2.01	0.42
1:P:2:GLU:N	3:P:2001:HOH:O	2.53	0.41
1:H:11:LYS:HB2	1:H:11:LYS:HE3	1.84	0.41
1:J:6:THR:HG22	1:J:117:MET:HG3	2.00	0.41
1:K:35:GLY:N	3:K:2017:HOH:O	2.54	0.41
1:B:9:TRP:O	3:B:2013:HOH:O	2.21	0.40
1:H:19:GLU:OE1	3:H:2017:HOH:O	2.22	0.40
1:I:99:GLU:HG2	3:I:2049:HOH:O	2.21	0.40
1:B:22:ARG:NH2	3:B:2043:HOH:O	2.46	0.40
1:G:46:HIS:CE1	1:G:113:HIS:HE1	2.39	0.40
1:P:10:LYS:HA	1:P:10:LYS:HD2	1.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2055:HOH:O	3:I:2026:HOH:O[2_656]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
1	B	121/125 (97%)	119 (98%)	2 (2%)	0	100	100
1	C	122/125 (98%)	121 (99%)	1 (1%)	0	100	100
1	D	121/125 (97%)	117 (97%)	4 (3%)	0	100	100
1	E	121/125 (97%)	119 (98%)	2 (2%)	0	100	100
1	F	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
1	G	121/125 (97%)	118 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	121/125 (97%)	118 (98%)	3 (2%)	0	100	100
1	I	121/125 (97%)	119 (98%)	2 (2%)	0	100	100
1	J	121/125 (97%)	117 (97%)	4 (3%)	0	100	100
1	K	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
1	L	122/125 (98%)	121 (99%)	1 (1%)	0	100	100
1	M	121/125 (97%)	116 (96%)	5 (4%)	0	100	100
1	N	122/125 (98%)	121 (99%)	1 (1%)	0	100	100
1	O	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
1	P	122/125 (98%)	121 (99%)	1 (1%)	0	100	100
All	All	1946/2000 (97%)	1908 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	102/102 (100%)	102 (100%)	0	100	100
1	B	100/102 (98%)	100 (100%)	0	100	100
1	C	101/102 (99%)	98 (97%)	3 (3%)	41	41
1	D	100/102 (98%)	99 (99%)	1 (1%)	76	81
1	E	100/102 (98%)	99 (99%)	1 (1%)	76	81
1	F	101/102 (99%)	100 (99%)	1 (1%)	76	81
1	G	100/102 (98%)	100 (100%)	0	100	100
1	H	100/102 (98%)	100 (100%)	0	100	100
1	I	100/102 (98%)	98 (98%)	2 (2%)	55	58
1	J	100/102 (98%)	99 (99%)	1 (1%)	76	81
1	K	102/102 (100%)	101 (99%)	1 (1%)	76	81
1	L	101/102 (99%)	99 (98%)	2 (2%)	55	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	100/102 (98%)	100 (100%)	0	100	100
1	N	101/102 (99%)	100 (99%)	1 (1%)	76	81
1	O	101/102 (99%)	100 (99%)	1 (1%)	76	81
1	P	101/102 (99%)	101 (100%)	0	100	100
All	All	1610/1632 (99%)	1596 (99%)	14 (1%)	78	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2	GLU
1	C	13	LYS
1	C	22	ARG
1	D	77	SER
1	E	15	VAL
1	F	13	LYS
1	I	2	GLU
1	I	100	LYS
1	J	13	LYS
1	K	97	LYS
1	L	22	ARG
1	L	103	LYS
1	N	22	ARG
1	O	100	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	5	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	123/125 (98%)	-0.40	0 100 100	20, 29, 47, 55	3 (2%)
1	B	123/125 (98%)	-0.38	0 100 100	21, 30, 47, 65	2 (1%)
1	C	124/125 (99%)	-0.44	0 100 100	20, 29, 43, 59	4 (3%)
1	D	123/125 (98%)	-0.37	1 (0%) 86 85	21, 30, 50, 65	1 (0%)
1	E	123/125 (98%)	-0.35	1 (0%) 86 85	20, 33, 51, 68	3 (2%)
1	F	123/125 (98%)	-0.35	0 100 100	22, 33, 48, 62	6 (4%)
1	G	123/125 (98%)	-0.29	0 100 100	23, 34, 53, 65	3 (2%)
1	H	123/125 (98%)	-0.30	0 100 100	23, 35, 56, 64	5 (4%)
1	I	123/125 (98%)	-0.43	0 100 100	16, 28, 47, 63	2 (1%)
1	J	123/125 (98%)	-0.47	0 100 100	20, 29, 46, 56	2 (1%)
1	K	123/125 (98%)	-0.38	0 100 100	19, 31, 48, 60	2 (1%)
1	L	123/125 (98%)	-0.41	0 100 100	18, 30, 47, 63	0
1	M	123/125 (98%)	-0.40	0 100 100	18, 31, 47, 55	1 (0%)
1	N	123/125 (98%)	-0.43	0 100 100	15, 28, 48, 55	2 (1%)
1	O	124/125 (99%)	-0.34	0 100 100	20, 32, 50, 65	0
1	P	123/125 (98%)	-0.35	0 100 100	21, 36, 55, 66	1 (0%)
All	All	1970/2000 (98%)	-0.38	2 (0%) 95 95	15, 31, 50, 68	37 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	11	LYS	2.4
1	D	23	ALA	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE2	F	201	1/1	0.96	0.08	31,31,31,31	0
2	FE2	H	201	1/1	0.97	0.06	30,30,30,30	0
2	FE2	P	201	1/1	0.98	0.05	35,35,35,35	0
2	FE2	B	201	1/1	0.98	0.08	31,31,31,31	0
2	FE2	N	201	1/1	0.99	0.09	21,21,21,21	0
2	FE2	E	201	1/1	0.99	0.05	25,25,25,25	0
2	FE2	C	201	1/1	0.99	0.04	25,25,25,25	0
2	FE2	J	201	1/1	0.99	0.09	26,26,26,26	0
2	FE2	G	201	1/1	0.99	0.08	24,24,24,24	0
2	FE2	M	201	1/1	0.99	0.05	25,25,25,25	0
2	FE2	O	201	1/1	0.99	0.07	26,26,26,26	0
2	FE2	D	201	1/1	0.99	0.05	27,27,27,27	0
2	FE2	K	201	1/1	1.00	0.10	27,27,27,27	0
2	FE2	A	201	1/1	1.00	0.05	21,21,21,21	0
2	FE2	L	201	1/1	1.00	0.07	29,29,29,29	0
2	FE2	I	201	1/1	1.00	0.10	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.